Position-space rescaling and hierarchical lattice models of disordered one-dimensional systems (invited)

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The application of exact and approximate position-space renormalization group techniques to the calculation of densities of states for problems with Gaussian generating functions (such as free tight-binding electrons, harmonic vibrations, spin waves, or random walks on Euclidian or "fractal" lattices) is briefly reviewed. It is also shown that for one-dimensional Gaussian theories with disorder, the approximate recursion relations proposed by Gonçalves da Silva and Koiller (GK) are exact for problems formulated on Berker–Ostlund lattices. A generalization of the GK scheme which allows one to calculate the optical zone-center density of states is formulated and then applied to the study of one- and two-mode behavior in mixed diatomic crystals.

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I. INTRODUCTION

Problems with linear "equations of motion," such as free electrons in the tight-binding approximation, harmonic chains, spin waves, or random walks, are usually trivial to solve unless they are formulated on special lattices such as fractals or unless disorder is present. Since exact renormalization group (RG) solutions can be written down in the easy cases, using the RG as a starting point for new approximation schemes in the more complicated cases holds the promise of new insights. This has been realized a while ago and quite a few ways to implement RG ideas have been explored.

In this paper, we first very briefly review the applications of a particular type of position-space RG which is analogous to decimation techniques in critical phenomena. Aoki, José, Sarker and Domany, and Wegner are among those who used such a technique to study the problem of Anderson localization. J. Machta has done extensive work in that spirit in the context of the random walk. None of the above work will be discussed in detail. We instead concentrate on more "mundane" density of states (DOS) problems which can be tackled in a manner analogous to that first suggested by Gonçalves da Silva and Koiller (GK). In the last part of this paper, we summarize the results we have obtained on the problem of, so-called, one- and two-mode behavior in mixed diatomic crystals. The appendix generalizes the proof of Langlois et al. concerning the connection between approximate recursion relations proposed by GK for disordered problems and exact solutions of problems formulated on hierarchical Berker–Ostlund lattices.

II. POSITION-SPACE RESCALING AND DOS

A. Exact results

In this section we discuss only systems with nonrandom distributions of physical parameters. To describe with a simple example the type of RG technique we have in mind, let us consider a chain of atoms of mass $M$ linked by harmonic forces with constant $K$. The Green's function at angular frequency $\omega$ is defined by

$$\sum_j [A_g - M_i (\omega^2 + i\eta)\delta_{ij}] G_{jk} = Z_{ik} M_k ,$$

where $Z_{ik} = \delta_{ik}$ is 1 for $i = k$ and zero otherwise while $\eta$ is a small positive number, and $A_g = 2K^{(0)}\delta_{ij} - L^{(0)}[\delta_{i+1,j} + \delta_{i-1,j}]$ with $L^{(0)} = K^{(0)}$. Consider the set of equations for, say, $G_{00}$. In the first step of the procedure, the lines with $j$ odd are eliminated; one is then left with half as many equations of motion with effective couplings which take the form

$$L^{(1)} = L^{(02)}/[2K^{(0)} - M(\omega^2 + \eta)] ,$$

and

$$K^{(1)} = K^{(0)} - L^{(1)} .$$

Changing the scale by a factor of two, the remaining equations take the same form as the original ones. Eq. (2) may thus be iterated until all degrees of freedom but one (i.e., $G_{00}$) are eliminated. It is important to note however that $K^{(n)}$ and $L^{(n)}$ are complex numbers and that for $\eta$ large enough convergence to $L^{(n)} = 0$ is reached before all degrees of freedom are eliminated. $\eta$ determines the precision with which each energy level is found. As usual the single site density of states (DOS) is obtained, for a chain with $N$ sites, from:

$$\rho_{\omega} (\omega^2) = \frac{1}{\pi} \text{Im} \left[ \frac{1}{L N} G_{00} \right] .$$

By allowing $Z_g$ to renormalize to something different from $\delta_g$, one can generalize the above renormalization group procedure in one dimension so as to compute either arbitrary correlation functions $G_g$ (which is usually not obtainable in the usual position-space RG) or to take into account interactions of arbitrary range. This has been discussed by South-
The latter generalization is particularly useful to tackle higher dimensional problems since in that case higher range interactions are generated by the decimation trick. Progress for this problem has been reported in Refs. 11 and 12.

All of the above problems may also be handled by Fourier transform techniques but numerically the decimation scheme may sometimes be more performant. If translational invariance is broken however, Fourier transforms are completely inadequate. When perfect dilation symmetry is preserved however, the above technique can still be very powerful to compute DOS. It has been used, for example, \cite{13,14} for problems defined on Sierpiński gaskets which are a special case of so-called “Fractal Lattices” \cite{15} for which renormalized interactions remain of short range in arbitrary dimension.

Finally, note that for all of the above problems, one can define a generating function, which is the analog of the free energy in critical phenomena, and from it one can extract analytically \cite{11,13} the scaling behavior of the DOS near fixed points of the RG transformation (e.g., the band edges for a one-dimensional nearest-neighbor problem).

B. Single-site density of states for disordered one-dimensional systems

It is relatively well known that the harmonic chain with a random binary distribution of masses and uniform spring constants has an extremely complicated spectrum. This problem has been studied at least since Dyson \cite{16} and quite a few exact results are also known. Much of the structure may be understood by considering small clusters of different sizes. \cite{17} Hence meanfield-like methods such as the coherent-potential-approximation (CPA) fail for disordered one-dimensional problems in that they predict very smooth spectra. \cite{18} RG methods by contrast, even approximate ones, which we then call rescalings, look at the problem on all length scales and hence may produce more acceptable results.

With the RG method described above, one can write down, even in the random case, formally exact recursion relations which eliminate $2N$ parameters in $\log_2N$ iterations. This procedure has been outlined by Southern et al. \cite{19} It is also useful to devise approximate schemes to perform faster calculations (which would allow to extend the technique to higher dimensions) and also to reduce the number of parameters in the hope of gaining insight into the problem.

To be specific, let us consider the binary harmonic chain problem mentioned above. After one iteration the effective “force constants” become random variables which one may describe by a probability distribution parametrized by a mean and a few moments. In 1981, Gonçalves da Silva and Koiller \cite{GK} proposed to simply keep the mean of that probability distribution, obtaining the following recursion relations when $c_A$ ($c_B$) is the probability of having a mass of type A (B) on a site:

$$L^{(1)} = L^{(0)} \left( A \right) \left( \begin{array}{c} \frac{L^{(0)}}{2K^{(0)} - M_A(\omega^2 + i\eta)} \\
+ c_B \frac{L^{(0)}}{2K^{(0)} - M_B(\omega^2 + i\eta)} \end{array} \right),$$

$$K^{(1)} = K^{(0)} - L^{(1)}.$$  \hspace{1cm} (4a)

Even though rather crude, this approximation has the following virtues: it does give a structured spectrum which shows even more structure as the energy resolution improves, like the exact DOS; it reproduces some of the exactly known gaps; \cite{20} it is exact in the small disorder limit $c_A \rightarrow 0$ or $c_B \rightarrow 1$; and it preserves the first three moments of the exact DOS. The latter fact has been demonstrated recently by Robbins and Koiller \cite{21} who also showed that the GK technique may be imagined as a virtual cluster approximation on renormalized Hamiltonians and hence may be extended to renormalized average-T-matrix or renormalized CPA schemes (respectively RATM and RCPM).

What is perhaps most surprising in the GK scheme is that it gives positive DOS. Indeed, if one tries to average something else than $K$ and $L$, \cite{22} one obtains DOS which are negative for certain energies. This positivity question has been considered in detail by Langlois et al. \cite{8} who proved this property formally from a generating function point of view and also, more interestingly, by showing that the GK recursion relations give the exact DOS of the central site of a so-called Berker–Ostlund \cite{9} hierarchical lattice. Such lattices were first proposed in the context of critical phenomena as an exact realization of approximate Migdal–Kadanoff recursion relations. The question then arises as to whether such hierarchical lattices may be used in statistical mechanics to study other problems with disorder. We show in the Appendix that for one-dimensional Gaussian-type problems, the equivalence between the GK rescaling scheme and exact solutions for Berker-Ostlund lattices holds. Note that these results provide a nice example of how an ordered but highly inhomogeneous fractal structure may serve as a model for a homogeneously disordered system. It indicates that in some sense, self-similarity under rescaling is a relevant “symmetry” of this type of problems.

As mentioned above, the GK scheme could be improved by keeping a parametrized probability distribution. This is the standard approach. Alternatively, as suggested by GK, one can keep only the mean of the probability distribution at the expense of having either (a) more complicated recursion relations obtained by eliminating more atoms before averaging over disorder, or (b) a larger parameter space obtained by keeping larger blocks of atoms as basic units of the scheme instead of single atoms. The exact limit is in principle reached in the latter case when one keeps large enough blocks. The motivation for this approach is that one wants to keep the essential simplicity of the scheme as well as its hierarchical lattice interpretation and verify to what extent it can be made into a realistic model of disorder. In case (b) that scheme may also be seen as a generalization of Cluster Bethe-lattice methods. \cite{23} The relative merits of these improvements as well as how one can extract information on the eigenvectors from the scaling trajectories has been discussed in detail by Langlois et al. \cite{8}.

In closing this section, we mention that by contrast with
As can be seen from Fig. 1, the results compare very well if the smallest size block which gives sensible results for the computer simulation results of Painter 35 on optical problems see Refs. 27 and 19. The GK technique has also been used in apparently unrelated contexts. 28

III. ONE-MODE TWO-MODE BEHAVIOR IN MIXED CRYSTALS

Mixed crystals of the type AB \(_{c}\) \(_{c}\) have one charged sublattice, A, which is ordered and another one of the opposite charge which is disordered (0 < c < 1). Roughly speaking, Raman spectra of such lattices may have in the disordered case, either a single mode whose frequency interpolates between the frequencies of the pure compound (c = 0 and c = 1) or two-modes of varying intensities which are more or less at the pure compound frequencies. Changes from one- to two-mode behavior as a function of c are also seen in certain compounds. This is a rather old subject which has been reviewed for example in 1971 by Chang and Mitra 29 and which still gets some experimental \(^{30,31}\) and theoretical \(^{22-34}\) attention. Even though one-dimensional mixed crystals exist, they have a more complicated unit cell than the one described above. Nevertheless, we first restrict ourselves to the simplest model and address two questions of interest. The first one is on the nature of eigenstates: are one-mode eigenstates more delocalized than two-mode eigenstates as one may expect? The second question regards the effect of long-range forces: do they tend to favor one type of behavior or the other? In the following paragraphs, we first sketch in words a generalization of the GK scheme which allows us to compute the zone-center (k = 0) optical-mode DOS and then present preliminary results on the subject. Details will appear elsewhere.

A. Method of calculation

We start from a generating function point of view \(^{22,8,13}\) and add to the argument of the exponentials terms proportional to \((- i \phi \sqrt{M})\) which couple linearly to the displacement variables on sites \(i\) and which are analog to the terms which appear in critical phenomena when a staggered magnetic field is applied. (See also the Appendix). The k = 0 optical DOS may then be obtained by taking the second derivative of the generating function with respect to \(\phi\). This allows recursion formulæ for that DOS to be written down directly.

To check the validity of the rescaling technique, we first compare our results for the average single site DOS with the computer simulation results of Painter \(^{35}\) on 20 000 atoms. In our case, the single site DOS is computed by first performing enough iterations that one is left with a single block with vanishing renormalized interactions with neighboring blocks. The single site DOS on that block are then averaged. As can be seen from Fig. 1, the results compare very well if one smooths out the histograms. The results in Fig. 1 are for blocks of eight atoms which, it turns out, seems to be the smallest size block which gives sensible results for the k = 0 optical DOS. Note that if one uses the average single site DOS of a single block of eight atoms, not attached to a hierarchical lattice (i.e., if no iterations are performed), then one does not obtain such good agreement with the computer simulations. The regions where the agreement between our results and the computer simulations is less satisfactory are away from the optical band edges which are of interest to us in this paper.

DOS at \(k = 0\) calculated by the method just described with blocks of eight atoms, do exhibit one- and two-mode behavior. In general however, the spectra are more structured than the experimentally observed ones, probably because the latter are obtained for systems which are not strictly one-dimensional.

The traditional classification between one- and two-mode behavior depends on a more or less subjective interpretation of experimental results for compounds which change from one- to two-mode behavior as a function of concentration. (That change is definitely not a phase transition!). Therefore, a complete comparison of theoretical and experimental spectra would definitely be more satisfactory. Nevertheless, in order to compare with previous theories and experimental results, we can establish a reasonable criterion to classify our spectra in the traditional way. Our results are not too sensitive to the precise form of this criterion. For the nearest-neighbor problem with uniform force constants, our results for the concentration dependent change from one- to two-mode behavior in the \(\beta = M_B / M_A\), \(\epsilon = 1 - M_C / M_B\) (\(M_C < M_B\)) plane are in qualitative agreement with the CPA results of Sen and Hartmann \(^{32}\) but disagree with those of Grünewald. \(^{32}\) For most mixed diatomic crystals both CPA and rescaling could be applied with success. For others, discrepancies can be attributed to higher dimensional effects or longer range forces (which we consider momentarily).

B. Localization of eigenstates

One finds that one-mode behavior generally corresponds to larger localization lengths than two-mode behav-
ior since for a given precision the convergence rate of the iterations for the DOS is slower in the former case.

One can also compute the average of \(|u_A|/|u_B|\) the ratio of displacements on sublattice A and on the other sublattice to verify how it differs from its value in the pure compounds \(M_{BI}/M_A\). In the one-mode case this ratio is usually larger than in the pure compound while it is smaller in the two-mode case.

Finally, the width of the one- and two-mode peaks is related to the lifetime and hence is interesting to compare.\(^{30}\) If we chose one- and two-mode systems at random we would obtain indifferently that either the one- or two-mode system has the largest width. To make a meaningful comparison, one must consider systems having equal optical bandwidths for their respective pure diatomic chains. For a one-mode compound with masses \(M_A = 1, M_B = x, M_C = y\), where \(x > y > 1\) and \(x^{-1} + y^{-1} < 1\), we must choose a corresponding two-mode system with masses \(M_A = y, M_B = x, M_C = 1\). In such a case, the one-mode systems are narrower, which is consistent with the idea that they are more delocalized, meaning that their projection on truly delocalized \(k = 0\) optical modes is closer to a delta function than in the case of a comparable two-mode compound.

C. Second nearest-neighbor forces

Nearest-neighbor theories of the type just described often fail to describe the behavior of group I–VII crystals such as RbCl, BrI, or BrK, RbCl. One-mode behavior is observed in these crystals while theory predicts two-mode behavior.\(^{34}\) Group I–VII crystals being ionic, long-range forces are certainly important. It is straightforward to include second-nearest-neighbor interactions \(K_2\) in the scheme described above. Results are exhibited in Fig. 2 for the case which is most favorable to the one-mode behavior and still corresponds to a stable system. The darker region is the one where one can prove rigorously from Saxon–Hutner\(^{30}\) type arguments with \(K_2/K_1 = -0.25\) that the behavior is two-mode. The right of the solid line is the corresponding area for nearest-neighbor forces only. The full calculation reveals that second-nearest-neighbor forces are not quite enough to account for the one-mode behavior of the compounds mentioned above. Clearly, longer range interactions or higher-dimensional effects may be needed. More importantly however, we have found that second-nearest-neighbor forces do not always favor one-mode behavior. On the contrary, for certain values of \(K_2/K_1\) the two-mode region is sometimes greatly enhanced. Further details and results will appear in a forthcoming publication.

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APPENDIX: GK APPROXIMATION VS HIERARCHICAL LATTICES

This appendix generalizes the results of Ref. 8. In general, let us consider one-dimensional problems such as harmonic vibrations, random walks etc., which have as their starting point generating functions of the form

\[ F = \ln \left( \int_{Du} e^{\sum_{i=1}^{N} H(u_i, \xi_i)} \right), \]  

(A1)

where

\[ \int_{Du} \equiv \int_{-\infty}^{\infty} \sum_{i=1}^{N} du_i, \]  

(A2)

and \(i\) runs over the \(N\) lattice sites. We restrict ourselves to a nearest-neighbor problem but it is easy to generalize the following results to interactions of range \(n\) by using, as basic units, vectors which include \(n\) sites (instead of one, as here). In general, the “Hamiltonian” in Eq. (1) takes the form

\[ H^{(0)}(u_i, \xi_{i+1}) = \frac{1}{2} \sum_{i} (\alpha^{(0)}_i u_i^2 + \alpha^{(0)}_{i+1} u_{i+1}^2 + \xi_i u_i + \xi_{i+1} u_{i+1}) + C^{(0)}_i + C^{(0)}_{i+1} + \beta^{(0)}_{i+1} u_i u_{i+1}, \]  

(A3)

where \(\alpha^{(0)}_i\) is a complex number whose real part is a small negative number which insures convergence of the integrals. \(C^{(0)}_i\) and \(C^{(0)}_{i+1}\) are constant terms which are in general generated by the rescaling transformation. Notice that single site terms have been divided equally between bonds [factor 1/2 in Eq. (A3)]. In general, \(\alpha_i, \beta_{i+1}\), and \(\xi_i\) are random variables which we assume independently distributed on each site or bond.

Let \(\mu_i\) be the set of indices necessary to describe a particular realization of the random parameters associated with site \(i\) or with the bonds attached to that site. Then let \(P(\mu_i)\) be

![Fig. 2: One- and two-mode behavior in the plane when the second-nearest-neighbor to first-nearest-neighbor force constant ratio is \(K_2/K_1 = -0.25\). All second-nearest-neighbor interactions are chosen identical. Change from one-mode, to the left, to two-mode behavior, to the right, occurs within the rescaling technique at the dotted line for \(c = 0.25\) and at the dashed line for \(c = 0.5\). The solid line is the Chang and Mitra criterion (Ref. 29) \(\beta < c/(1 - c)\) for \(K_2 = 0\) and the dark region is the corresponding criterion, \(\beta < (c - 1/2)/(1 - c)\), when \(K_2/K_1 = -0.25\).](image-url)
the probability distribution for site $i$:

$$P(\mu_i) > 0; \sum_\mu P(\mu_i) = 1.$$  \hfill (A4)

In the GK method, one first eliminates one site out of two to obtain the exact effective "Hamiltonian,"

$$\sum_{\text{odd}} H^{(1)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_{i+1})$$

$$= \ln \left\{ \prod_{\mu_i} \int du_i \exp \left[ H^{(0)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_i) \right. \right.$$

$$\left. + H^{(0)}_{\mu_i, \mu_{i+1}}(u_i, u_{i+1}) \right\}.$$  \hfill (A5)

The approximate step of the GK approach is to force the probability distribution back to its original form by immediately averaging Eq. (A5) over the disorder associated with the eliminated sites, i.e.,

$$\sum_{\text{odd}} \tilde{H}^{(1)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_{i+1})$$

$$= \sum_{\text{odd}} P(\mu_i) H^{(1)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_{i+1}).$$  \hfill (A6)

Notice that in the case of bond disorder, one must average with respect to the bond on only one of the two sides of the eliminated site, otherwise all disorder disappears at the first iteration, contrarily to the spirit of the GK approach. Equating the coefficients of the various polynomials in $u_i$, one obtains simple recursion relations for the parameters $a_i$, $\beta_{i+1}$, $C_i$, $\tilde{2}_i$. Because of the averaging procedure, the odd sites on either side of an uneliminated even site give equal contributions to the renormalized $a_i$. Hence the recursion relations for the renormalized parameters may also be found from

$$\tilde{H}^{(1)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_{i+1})$$

$$= \ln \left\{ \prod_{\mu_i} \int du_i \exp \left[ H^{(0)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_i) \right.$$

$$\left. + H^{(0)}_{\mu_i, \mu_{i+1}}(u_i, u_{i+1}) \right\} P(\mu_i),$$  \hfill (A7)

which follows from the above remark and from Eqs. (A5) and (A6). The same recursion relations for the renormalized parameters may also be obtained from the following equation:

$$\tilde{H}^{(1)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_{i+1})$$

$$= \ln \left\{ \prod_{\mu_i} \int du_i \exp \left[ P(\mu_i) H^{(0)}_{\mu_i^{-1}, \mu_i, \mu_{i+1}}(u_{i-1}, u_i) \right.$$

$$\left. + P(\mu_i) H^{(0)}_{\mu_i, \mu_{i+1}}(u_i, u_{i+1}) \right\}.$$  \hfill (A8)

To show that, it suffices to use the following results:

$$I_1 = \left( \int_{-\infty}^{\infty} du_1 \exp \left[ -au_1^2 + bu_1 + c \right] \right)^N$$

$$= \sqrt{\pi/\alpha} \exp \left[ \gamma c + \gamma b^2/(4\alpha) \right],$$  \hfill (A9a)

$$I_2 = \int_{-\infty}^{\infty} du_i \exp \left[ \gamma( -au_i^2 + bu_i + c) \right]$$

$$= \sqrt{\pi/\alpha} \exp \left[ \gamma c + \gamma b^2/(4\alpha) \right].$$  \hfill (A9b)

Only the prefactors are different in Eqs. (A9a) and (A9b) and since only the analogs of $\ln I_1$ and $\ln I_2$ are involved in Eqs. (A7) and (A8) this means that the recursion for the constant term $C$ is the only one that may differ in Eqs. (A7) and (A8). Since the constant term $C$ is not necessary to find the single site Green's function while for the optical zone-center DOS derivatives with respect to $\phi = (|s_i|/M)^{1/2}$ do not involve the prefactor, then one may use either Eq. (A8) or Eq. (A7) to generate the GK recursion relations.

Eq. (A8) will be used to show the equivalence to a problem formulated on a hierarchical lattice. Note first that as usual length rescaling maps the problem into the original one after each iteration, hence Eqs. (A7) and (A8) hold in general with $H^{(n)}$ on the left-hand side and $H^{(n-1)}$ on the right-hand side. Suppose we have a finite chain of length $2 \times 2^n$ for which all degrees of freedom except the central one and those of the two ends can be eliminated after $n$ iterations. Neglecting, for simplicity, the fact that the last iteration may differ from the other ones depending on the boundary conditions, we notice that $H^{(n)}$ in Eq. (A8) [Fig. 3(a)] may be obtained from the lattice illustrated in Fig. 3(b).

To understand Fig. 3, note also that single site terms which do not depend on the eliminated degrees of freedom (sites $0$ and $\pm 2^n$) can be factored out from the product on the right-hand side of Eq. (A8). Hence, no factors of $p$ or $(1 - p)$ appear for these sites because of the property Eq. (A4).

To continue this process, notice first that if the left-hand side of Eq. (A8) is multiplied by $p$, for example, then

$$\sqrt{\pi/\alpha} \exp \left[ \gamma c + \gamma b^2/(4\alpha) \right].$$

FIG. 3. Open circles represent single site parameters and straight lines represent nearest-neighbor interactions in the effective Hamiltonians. The lower index of $a^{n-1}$ specifies, for a binary distribution, which of the two possible values this parameter takes at that site. If no number is indicated, one can choose one value or the other for that parameter at will. The numbers on top of part (a) indicate the length scale in units of the original lattice spacing.

Upon iteration, one finds the parameters of Fig. 3(a) from Fig. 3(b).
FIG. 4. Elimination of the sites on the finest scale on this figure lead to Fig. 3(b). Enough labels have been written to allow the reader to generalize for himself.

using the same identity as that which led from Eq. (A7) to Eq. (A8), one finds that the “Hamiltonians” on the right-hand side of Eq. (A8) are multiplied by the same factor. Hence, the lattice of Fig. 4 does lead to the $p \alpha (n - 1)$ etc. of Fig. 3(b). Repeating this process, one finally works his way to $H^{(0)}$ and finds the complete hierarchical lattice for which the recursion relations are exact.

Alternatively, one can start from this hierarchical lattice and recover the GK recursion relations by using the converse of the properties just mentioned: (a) constant factors multiplying the Hamiltonians on both sides of Eq. (A8) may be simplified, and (b) single site terms which are not eliminated at a given iteration may be divided among “bonds” with appropriate multiplicative factors of $p$ and $(1 - p)$.


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